

In₃Se₄ Structure:

A3B4_hR7_166_ac_2c-001

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<https://aflow.org/prototype-encyclopedia/DJRQ>

https://aflow.org/prototype-encyclopedia/A3B4_hR7_166_ac_2c-001

Prototype	In ₃ Te ₄
AFLOW prototype label	A3B4_hR7_166_ac_2c-001
ICSD	44655
CCDC	1614010
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B4_hR7_166_ac_2c-001 --params=a, c/a, x₂, x₃, x₄</code>

Other compounds with this structure

Bi₃Te₄, Fe₃S₄ (smythite), In₃Se₄

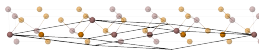
- (Geller, 1965) created this structure under pressures of about 35 kBar, but works such as (Villars, 2018) list it as the room temperature structure for In₃Te₄.
- In₃Te₄ and Sn₄P₃ have the same AFLOW prototype label, A3B4_hR7_166_ac_2c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

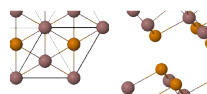
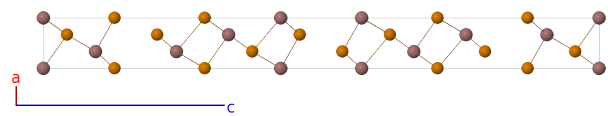
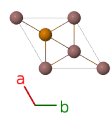
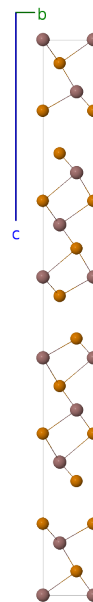
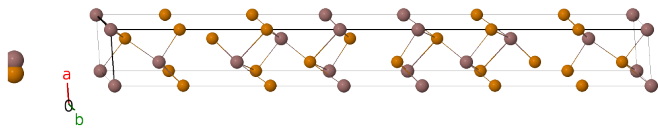
$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$$



In
Te



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) In I
$\mathbf{B}_2$	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$cx_2 \hat{\mathbf{z}}$	(2c) In II
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-cx_2 \hat{\mathbf{z}}$	(2c) In II
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$cx_3 \hat{\mathbf{z}}$	(2c) Te I
$\mathbf{B}_5$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-cx_3 \hat{\mathbf{z}}$	(2c) Te I
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$cx_4 \hat{\mathbf{z}}$	(2c) Te II
$\mathbf{B}_7$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-cx_4 \hat{\mathbf{z}}$	(2c) Te II

References

- [1] S. Geller, A. Jayaraman, and J. G. W. Hull, *Crystal chemistry and superconductivity of pressure-induced phases in the In-Te system*, J. Phys. Chem. Solids **26**, 353–361 (1965), doi:10.1016/0022-3697(65)90164-2.
- [2] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Indium-Tellurium Binary Phase Diagram (1998 Budanova N.Y.). Copyright ©2006-2018 ASM International.

Found in

- [1] G. Han, Z.-G. Chen, C. Sun, L. Yang, L. Cheng, Z. Li, W. Lu, Z. M. Gibbs, G. J. Snyder, K. Jack, J. Drennan, and J. Zou, *A new crystal: layer-structured rhombohedral In₃Se₄*, CrystEngComm **16**, 393–398 (2014), doi:10.1039/c3ce41815d.

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